On local invariants of pure three-qubit states

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Abstract

We study invariants of three-qubit states under local unitary transformations, i.e. functions on the space of entanglement types, which is known to have dimension 6. We show that there is no set of six independent polynomial invariants of degree ≤ 6, and find such a set with maximum degree 8. We describe an intrinsic definition of a canonical state on each orbit, and discuss the (non-polynomial) invariants associated with it.

1 Introduction

The invariants of many-particle states under unitary transformations which act on single particles separately ("local" transformations) are of interest [8, 9, 1, 6, 5, 10] because they give the finest discrimination between different types of entanglement. They can be regarded as coordinates on the space of entanglement types, (equivalently, the space of orbits of the group of local transformations). In this paper we study the case of pure states of three spin-$\frac{1}{2}$ particles, or qubits. For mixed states of two qubits, it is possible to give a complete set of invariants [13], describing the 9-dimensional space of orbits in terms of 14 invariants subject to 5 relations. For pure three-qubit states, where the space of orbits is known [1, 5] to be 6-dimensional, we can at present do no more than find a set of six independent invariants. We will show (Section 3) that in order to do this with polynomials in the state coordinates it is necessary to go to polynomials of order 8, and we will exhibit (Section 4) a set of six independent invariants all of which have a physical meaning. We will also discuss (Section 5) the possibility of finding a more convenient set of non-polynomial invariants. Section 2 is an introductory discussion of the invariants of pure n-qubit states.

2 Pure states: general considerations

A general theory of local invariants of mixed n-particle states has been given by Rains and Grassl et al. [6, 10]. Here we give the corresponding theory for the simpler case of pure states.

The most general system is that of n non-identical particles $A, B, \dots$ with one-particle state spaces of dimensions $d_A, d_B, \dots$. Let $|\psi_i^X\rangle : i = 1, \dots, d_X\}$ be an orthonormal basis of one-particle states of particle X; then the general n-particle state can be written

$$|\Psi\rangle = \sum_{ijk\cdots} t^{ijk\cdots} |\psi_i^{(A)}\rangle |\psi_j^{(B)}\rangle |\psi_k^{(C)}\rangle \cdots$$

where the sum is over values of i from 1 to d_A, values of j from 1 to d_B, and so on. By the First Fundamental Theorem of invariant theory [14], any polynomial in $t^{ijk\cdots}$ which is invariant under the action on $|\Psi\rangle$ of the local group $U(d_A) \times U(d_B) \times \cdots$ is a sum of homogeneous polynomials of even degree (say $2r$), of the form

$$I_{\sigma\tau\cdots}(t) = t^{i_1 j_1 k_1 \cdots} \cdots t^{i_r j_r k_r \cdots} \bar{t}_{i_1 j_{\sigma(1)} k_{\tau(1)} \cdots} \cdots \bar{t}_{i_r j_{\sigma(r)} k_{\tau(r)} \cdots} \qquad (2.1)$$

where $\sigma, \tau, \dots$ are permutations of $(1, \dots, r)$. Here $\overline{t}_{ijk\cdots}$ is the complex conjugate of $t^{ijk\cdots}$, and we adopt the usual summation convention on repeated indices, one in the upper position and one in the lower. Note that $P_{\sigma\tau\cdots}$ is unchanged by simultaneous conjugation of the permutations $\sigma, \tau, \dots$:

$$P_{\sigma\tau\cdots}(t) = P_{\sigma'\tau'\cdots}(t) \quad \text{if} \quad \sigma' = \kappa\sigma\kappa^{-1}, \quad \tau' = \kappa\tau\kappa^{-1}, \quad \dots$$

since such a conjugation merely expresses the effect of changing the order of the factors in P.

For two particles A, B there is just one permutation σ, which we can decompose into cycles $\kappa_1, \dots, \kappa_s$ of lengths $l_1, \dots, l_s$ with $l_1 + \cdots + l_s = r$. The polynomial $P_\sigma(t)$ then splits into a product of polynomials $P_{\kappa_1} \cdots P_{\kappa_s}$, where P_κ depends only on the length of the cycle κ, which is equal to half the degree of P_κ:

$$\begin{aligned} P_\kappa(t) &= t^{i_1 j_1} \overline{t}_{i_1 j_{\kappa(1)}} t^{i_{\kappa(1)} j_{\kappa(1)}} \overline{t}_{i_{\kappa(1)} j_{\kappa^2(1)}} \cdots \\ &= t^{i_1 j_1} \overline{t}_{i_1 j_2} t^{i_2 j_2} \overline{t}_{i_2 j_3} \cdots t^{i_l j_l} \overline{t}_{i_l j_1} \end{aligned}$$

(by renaming the dummy indices $j_{\kappa(1)}, j_{\kappa^2(1)}, \dots, j_{\kappa^{l-1}(1)}$)

$$= \mathrm{tr}(\rho_B^l)$$

where $\rho_B = \mathrm{tr}_A \, |\Psi\rangle\langle\Psi|$ is the density matrix of particle B, with matrix elements

$$(\rho_B)^j_k = t^{ij} \overline{t}_{ik}.$$

Thus the polynomial invariants of a two-particle pure state are the sums of the powers of the eigenvalues of ρ. These can all be expressed in terms of the first d_B power-sums, which generate the algebra of invariant polynomials and are independent if the eigenvalues are independent. However, they are not independent if $d_A < d_B$, for in that case some of the eigenvalues of ρ vanish. But clearly the same argument could be used to show that the algebra of invariants is generated by the traces of the powers of ρ_A, which is consistent because the non-zero eigenvalues of ρ_A are the same as those of ρ. Thus the algebra of polynomial invariants of two-particle pure states has a set of independent generators

$$\mathrm{tr}(\rho_A^l) = \mathrm{tr}(\rho^l), \qquad l = 1, \dots, \min(d_A, d_B).$$

The non-zero eigenvalues of ρ_A (or ρ) are in fact the squares of the coefficients in the Schmidt decomposition of $|\Psi\rangle$, so what we have here is the well-known fact that the local invariants of a pure two-particle state are the symmetric functions of the Schmidt coefficients.

3 Polynomial invariants of three-qubit states

For the remainder of the paper we consider three spin-$\frac{1}{2}$ particles A, B, C. The classification of pure states of this system has been discussed in [12, 4, 2], and their invariants in [5, 7, 3]. It is known [8] that the dimension of the space of orbits is 6; there are therefore six independent local invariants. We will show that there are no more than five independent invariants of degree less than 8, and exhibit a set of six independent invariants with maximum degree 8 [1].

The vector space of invariants of degree r is spanned by functions $P_{\sigma\tau}$ labelled by pairs of elements of S_r, the group of permutations of r things. Thus there is one independent invariant of degree 2,

$$I_1 = P_{ee}(t) = t^{ijk}\bar{t}_{ijk} = \langle\Psi|\Psi\rangle$$

where e is the identity permutation, so that $S_1 = \{e\}$. If $S_2 = \{e, \sigma\}$, the four linearly independent quartic invariants are

$$\begin{aligned} P_{ee}(t) &= t^{i_1j_1k_1}\bar{t}_{i_1j_1k_1}t^{i_2j_2k_2}\bar{t}_{i_2j_2k_2} = \langle\Psi|\Psi\rangle^2, \\ I_2 = P_{e\sigma}(t) &= t^{i_1j_1k_1}\bar{t}_{i_1j_1k_2}t^{i_2j_2k_2}\bar{t}_{i_2j_2k_1} = \mathrm{tr}(\rho_C^2), \\ I_3 = P_{\sigma e}(t) &= t^{i_1j_1k_1}\bar{t}_{i_1j_2k_1}t^{i_2j_2k_2}\bar{t}_{i_2j_1k_2} = \mathrm{tr}(\rho_B^2), \\ I_4 = P_{\sigma\sigma}(t) &= t^{i_1j_1k_1}\bar{t}_{i_1j_2k_2}t^{i_2j_2k_2}\bar{t}_{i_2j_1k_1} = \mathrm{tr}(\rho_A^2) \end{aligned}$$

where ρ_A, ρ_B, ρ_C are the one-particle density matrices:

$$\rho_X = \mathrm{tr}_{YZ}\,|\Psi\rangle\langle\Psi| \text{ where } \{X, Y, Z\} = A, B, C \text{ in some order.}$$

Thus there are at most four algebraically independent invariants of degree ≤ 4.

Higher-order invariants $P_{\pi\sigma}(t)$ with $\pi, \sigma \in S_3$ are functions of the four quadratic and quartic invariants if π and σ are equal or if either of them is the identity. To see this, note first that if $\pi = \sigma$,

$$\begin{aligned} P_{\sigma\sigma}(t) &= t^{i_1j_1k_1}\cdots t^{i_rj_rk_r}\bar{t}_{i_1j_{\sigma(1)}k_{\sigma(1)}}\cdots\bar{t}_{i_rj_{\sigma(r)}k_{\sigma(r)}} \\ &= (\rho_A)^{i_1}_{i_{\tau(1)}}(\rho_A)^{i_1}_{i_{\tau(2)}}\cdots(\rho_A)^{i_r}_{i_{\tau(r)}} \end{aligned}$$

where $\tau = \sigma^{-1}$. This is a product of traces of powers of ρ_A. But since ρ_A is a 2×2 matrix, the Cayley-Hamilton theorem enables us to express $\mathrm{tr}(\rho_A^r)$ for $r \geq 3$ as a function of $\mathrm{tr}\,\rho_A$ and $\mathrm{tr}\,\rho_A^2$.

[1] I understand that similar conclusions have been reached by Grassl [5]

Secondly, if $\pi = e$,

$$\begin{aligned} P_{e\sigma}(t) &= t^{i_1j_1k_1}\cdots t^{i_rj_rk_r}\overline{t}_{i_1j_1k_{\sigma(1)}}\cdots\overline{t}_{i_rj_rk_{\sigma(r)}} \\ &= (\rho)^{k_1}_{k_{\sigma(1)}}\cdots(\rho)^{k_r}_{k_{\sigma(r)}} \end{aligned}$$

which is a product of traces of powers of ρ; and similarly $P_{\pi e}(t)$ is a product of traces of powers of ρ.

Thus the only sextic invariants $P_{\pi\sigma}$ which are independent of the quadratic and quartic invariants are those for which π and σ are distinct 2-cycles, or distinct 3-cycles, or one is a 2-cycle and the other is a 3-cycle. Moreover, in each of these categories all the possible pairs (π, σ) are related by simultaneous conjugation and therefore give the same invariant. There are therefore three possible independent sextic invariants:

1. π, σ distinct 3-cycles, say $\pi = (123)$, $\sigma = (132)$. This gives

$$\begin{aligned} I_5 = P_{(123)(132)}(t) &= t^{i_1j_1k_1}t^{i_2j_2k_2}t^{i_3j_3k_3}\overline{t}_{i_1j_2k_3}\overline{t}_{i_2j_3k_1}\overline{t}_{i_3j_1k_2} \\ &= (\rho_{BC})^{j_1k_1}_{j_2k_3}(\rho_{BC})^{j_2k_2}_{j_3k_1}(\rho_{BC})^{j_3k_3}_{j_1k_2} \end{aligned} \tag{3.1}$$

where $\rho_{BC} = \mathrm{tr}_1\,|\Psi\rangle\langle\Psi|$ is the density matrix of the two-particle system of particles 2 and 3. This invariant was identified by Kempe [7] as one which distinguishes three-particle states which have identical density matrices for every subsystem. It has exactly the same form when expressed as a function of ρ_{AB} or of ρ_{AC}.

2. π, σ distinct 2-cycles, say $\pi = (12)$, $\sigma = (23)$. This gives

$$\begin{aligned} I_5' = P_{(12)(23)}(t) &= t^{i_1j_1k_1}t^{i_2j_2k_2}t^{i_3j_3k_3}\overline{t}_{i_1j_2k_1}\overline{t}_{i_2j_1k_3}\overline{t}_{i_3j_3k_2} \\ &= (\rho_B)^{j_1}_{j_2}(\rho_C)^{k_3}_{k_2}(\rho_{BC})^{j_2k_2}_{j_1k_3} \\ &= \mathrm{tr}(\rho_B\rho_C\rho_{BC}), \end{aligned} \tag{3.2}$$

identifying ρ_B with $\rho_B \otimes \mathbf{1}$ as an operator on states of particles 2 and 3, and similarly ρ_C with $\mathbf{1} \otimes \rho_C$.

3. π a 2-cycle, say (12), and σ a 3-cycle, say (123), or vice versa. These give

$$\begin{aligned} I_5'' = P_{(12)(123)}(t) &= t^{i_1j_1k_1}t^{i_2j_2k_2}t^{i_3j_3k_3}\overline{t}_{i_1j_2k_2}\overline{t}_{i_2j_1k_3}\overline{t}_{i_3j_3k_1} \\ &= (\rho_{AC})^{i_1k_1}_{i_2k_3}(\rho_A)^{i_2}_{i_1}(\rho_C)^{k_3}_{k_1} \\ &= \mathrm{tr}(\rho_A\rho_C\rho_{AC}) \end{aligned} \tag{3.3}$$

and

$$\begin{aligned} I_5''' = P_{(123)(12)}(t) &= t^{i_1j_1k_1}t^{i_2j_2k_2}t^{i_3j_3k_3}\overline{t}_{i_1j_2k_2}\overline{t}_{i_2j_3k_1}\overline{t}_{i_3j_1k_3} \\ &= \mathrm{tr}(\rho_A\rho_B\rho_{AB}). \end{aligned} \tag{3.4}$$

Primes have been placed on the symbols for these last three invariants because they will not feature in our final list of independent invariants, each of them being expressible in terms of I_5 and the quadratic and quartic invariants. To show this, we write I_5 in terms of 2×2 matrices by considering the 4×4 matrix ρ_{BC} as a set of four 2×2 matrices $X^{j_1}_{j_2}$: the matrix elements of $X^{j_1}_{j_2}$, labelled by (k_1, k_2), are

$$(X^{j_1}_{j_2})^{k_1}_{k_2} = (\rho)^{j_1 k_1}_{j_2 k_2}.$$

Then

$$I_5 = \mathrm{tr}(X^{j_1}_{j_2} X^{j_3}_{j_1} X^{j_2}_{j_3}).$$

Now we use the 2×2 matrix identity

$$\begin{aligned} \mathrm{tr}(XYZ) + \mathrm{tr}(XZY) = \mathrm{tr}\, X \,\mathrm{tr}(YZ) + \mathrm{tr}\, Y \,\mathrm{tr}(ZX) + \mathrm{tr}\, Z \,\mathrm{tr}(XY) \\ - \mathrm{tr}\, X \,\mathrm{tr}\, Y \,\mathrm{tr}\, Z \end{aligned} \tag{3.5}$$

which holds for any 2×2 matrices X, Y, Z, and can be obtained by linearising the cubic identity

$$\mathrm{tr}\, X^3 = \tfrac{3}{2} \,\mathrm{tr}\, X \,\mathrm{tr}\, X^2 - \tfrac{1}{2} (\mathrm{tr}\, X)^3$$

which in turn is obtained by taking the trace of the Cayley-Hamilton theorem. Apply (3.5) to the matrices $X^{j_1}_{j_2}$, $X^{j_3}_{j_1}$, $X^{j_2}_{j_3}$ occurring in the expression for I_5. The first term on the left-hand side is I_5; the second is

$$\mathrm{tr}(X^{j_1}_{j_2} X^{j_2}_{j_3} X^{j_3}_{j_1}) = \mathrm{tr}(\rho_{BC}^3) = \mathrm{tr}(\rho_A^3)$$

since the non-zero eigenvalues of ρ_{BC} are the same as those of ρ_A (both being the squares of the coefficients in a Schmidt decomposition of $|\Psi\rangle$)). The first term on the right-hand side is

$$\begin{aligned} \mathrm{tr}(X^{j_1}_{j_2}) \,\mathrm{tr}(X^{j_3}_{j_1} X^{j_2}_{j_3}) &= (\sigma)^{j_1}_{j_2} (\rho_{BC})^{j_3 k_1}_{j_1 k_2} (\rho_{BC})^{j_2 k_2}_{j_3 k_1} \\ &= (\sigma)^{j_1}_{j_2} t^{i_1 j_3 k_1} \bar{t}_{i_1 j_1 k_2} t^{i_2 j_2 k_2} \bar{t}_{i_2 j_3 k_1} \\ &= (\sigma)^{j_1}_{j_2} (\rho_A)^{i_1}_{i_2} (\rho_{AB})^{i_2 j_2}_{i_1 j_1} \\ &= \mathrm{tr}(\rho_A \rho_B \rho_{AB}); \end{aligned}$$

the second and third terms differ from the first only by permuting the indices j_1, j_2, j_3 and therefore (after summing) are equal to it; and the last term is

$$\mathrm{tr}(X^{j_1}_{j_2}) \,\mathrm{tr}(X^{j_2}_{j_3}) \,\mathrm{tr}(X^{j_3}_{j_1}) = \mathrm{tr}(\sigma^3).$$

Thus (3.5) gives

$$I_5 = 3\,\mathrm{tr}(\rho_A\rho_B\rho_{AB}) - \mathrm{tr}(\rho_A^3) - \mathrm{tr}(\rho^3). \tag{3.6}$$

Similarly, using the alternative expressions for I_5 in terms of ρ_{AB} and ρ_{AC} gives

$$\begin{aligned} I_5 &= 3\,\mathrm{tr}(\rho_B\rho_C\rho_{BC}) - \mathrm{tr}(\rho_B^3) - \mathrm{tr}(\rho^3) &(3.7)\\ &= 3\,\mathrm{tr}(\rho_A\rho_C\rho_{AC}) - \mathrm{tr}(\rho_A^3) - \mathrm{tr}(\rho_C^3). &(3.8)\end{aligned}$$

So there are at most five independent invariants of degree 6 or less. Since six invariants are needed to parametrise the orbits [8], we must use at least one invariant of degree 8 or more. A convenient, and physically significant, choice is the 3-tangle identified by Coffman, Kundu and Wootters [3]:

$$I_6 = \tfrac{1}{4}\tau_{123}^2 = \left|\epsilon_{i_1i_2}\epsilon_{i_3i_4}\epsilon_{j_1j_2}\epsilon_{j_3j_4}\epsilon_{k_1k_3}\epsilon_{k_2k_4}t^{i_1j_1k_1}t^{i_2j_2k_2}t^{i_3j_3k_3}t^{i_4j_4k_4}\right|^2 \tag{3.9}$$

where ϵ_{ij} is the antisymmetric tensor in two dimensions ($\epsilon_{12} = -\epsilon_{21} = 1$, $\epsilon_{11} = \epsilon_{22} = 0$). The expression between the modulus signs is an $\mathrm{SU}(2)^3$ invariant (though not a $\mathrm{U}(2)^3$ invariant — its phase is not invariant under local transformations), so its modulus is a local invariant. The invariant I_6 can be put into our standard form (2.1) by multiplying the $\mathrm{SU}(2)^3$ invariant by its complex conjugate

$$\epsilon^{i_5i_6}\epsilon^{i_7i_8}\epsilon^{j_5j_6}\epsilon^{j_7j_8}\epsilon^{k_5k_7}\epsilon^{k_6k_8}\bar{t}_{i_5j_5k_5}\bar{t}_{i_6j_6k_6}\bar{t}_{i_7j_7k_7}\bar{t}_{i_8j_8k_8}$$

(where the contravariant tensor ϵ^{ij} is numerically the same as ϵ_{ij}), and using the identity

$$\epsilon^{ab}\epsilon_{cd} = \delta^a_c\delta^b_d - \delta^a_d\delta^b_c.$$

To show that the invariants $I_1, \ldots, I_6$ are independent it is sufficient to show that their gradients are linearly independent at some point. We can treat t^{ijk} and $\bar{t}_{ijk}$ formally as independent coordinates in the 16 (real) - dimensional space of pure states, and we need only consider derivatives with respect to t^{ijk}, since independence of these 8-component vectors $\partial_t I_a$ will imply independence of the full 16-dimensional gradient vectors. The results of calculating $\partial I_a/\partial t^{ijk}$ and putting

$$t^{001} = t^{011} = t^{100} = t^{101} = 1, \quad t^{000} = t^{010} = t^{110} = t^{111} = 0, \quad \bar{t}_{ijk} = t^{ijk},$$

(where 0 and 1 are the two possible values of i, j, k) are as follows:

$$
\begin{aligned}
\partial_t I_1 &= (0,1,0,1,1,1,0,0) \\
\partial_t I_2 &= (2,6,2,6,4,6,0,0) \\
\partial_t I_3 &= (0,6,0,2,6,6,2,2) \\
\partial_t I_4 &= (2,6,0,2,6,6,0,2) \\
\partial_t I_5 &= (9,27,3,15,15,27,0,9) \\
\partial_t I_6 &= (0,0,4,-4,-4,0,4,0)
\end{aligned}
$$

These six vectors are indeed linearly independent.

4 Canonical coordinates

An alternative type of invariant, not necessarily a polynomial in the coordinates of the state vector, is obtained by specifying a canonical point on each orbit. The values of the invariant functions at any point are then the coordinates of the canonical point on its orbit. The canonical points lie on a manifold corresponding to the space of orbits, and their coordinates can (at least locally) be expressed in terms of an appropriate number of parameters.

One form of canonical state was suggested independently by Linden and Popescu [8] and by Schlienz [11], who pointed out that any pure state of three qubits can be written as

$$
\begin{aligned}
|\Psi\rangle = &\cos\theta|0\rangle\left(\cos\phi|0\rangle|0\rangle + \sin\phi|1\rangle|1\rangle\right) \\
&+ \sin\theta|1\rangle\left(r(-\sin\phi|0\rangle|0\rangle + \cos\phi|1\rangle|1\rangle) + s|0\rangle|1\rangle + te^{i\omega}|1\rangle|0\rangle\right)
\end{aligned}
\tag{4.1}
$$

where $0 \le \theta, \phi \le \pi/4,\ 0 \le \omega < 2\pi$ and r, s, t are non-negative real numbers satisfying $r^2 + s^2 + t^2 = 1$.

It is straightforward to calculate the invariants $I_1, \dots, I_6$ in terms of the Linden-Popescu-Schlienz parameters; the results are not enlightening. We will now describe another, more intrinsically defined, form of canonical point whose coordinates are more simply related to $I_1, \dots, I_6$.

The three-particle state $|\Psi\rangle$ has three Schmidt decompositions:

$$
\begin{aligned}
|\Psi\rangle &= \sum_i \alpha_i|\phi_i\rangle_A|\Phi\rangle_{BC} \\
&= \sum_i \beta_i|\theta_i\rangle_B|\Theta_i\rangle_{AC} \\
&= \sum_i \gamma_i|\chi_i\rangle_C|X_i\rangle_{AB}
\end{aligned}
\tag{4.2}
$$

where $\{|\phi_i\rangle\}$, $\{|\theta_i\rangle\}$ and $\{|\chi_i\rangle\}$ $(i = 0, 1)$ are orthonormal pairs of one-particle states, $\{|\Phi_i\rangle\}$, $\{|\Theta_i\rangle\}$ and $\{|X_i\rangle\}$ are orthonormal pairs of two-particle states, the suffices indicate which of the three particles A, B, C are in which state, and $\{\alpha_i\}$, $\{\beta_i\}$ and $\{\gamma_i\}$ are pairs of non-negative real numbers satisfying

$$\alpha_1^2 + \alpha_2^2 = \beta_1^2 + \beta_2^2 = \gamma_1^2 + \gamma_2^2 = \langle\Psi|\Psi\rangle = I_1. \tag{4.3}$$

These Schmidt coefficients, being the positive square roots of the eigenvalues of the one-particle density matrices ρ_A, ρ_B, ρ_C, are related to the quartic eigenvalues by

$$\begin{aligned} \alpha_1^4 + \alpha_2^4 &= \mathrm{tr}(\rho_A^2) = I_2, \\ \beta_1^4 + \beta_2^4 &= \mathrm{tr}(\rho_B^2) = I_3, \\ \gamma_1^4 + \gamma_2^4 &= \mathrm{tr}(\rho_C^2) = I_4. \end{aligned} \tag{4.4}$$

These equations have unique real non-negative solutions for $\alpha_i, \beta_i, \gamma_i$ provided the invariants $I_1, \ldots, I_4$ satisfy

$$I_1 > 0, \qquad \tfrac{1}{2}I_1^2 \leq I_2, I_3, I_4 \leq I_1^2.$$

Now consider the coordinates c^{ijk} of $|\Psi\rangle$ with respect to the canonical basis $|\phi_i\rangle_A|\theta_j\rangle_B|\chi_k\rangle_C$. If the states $|\phi_i\rangle, |\theta_j\rangle, |\chi_k\rangle$ were uniquely determined by $|\Psi\rangle$ — and they almost are — then the coordinates c^{ijk} would be local invariants. However, the Schmidt decompositions do not determine the phases of $|\phi_i\rangle$, $|\theta_j\rangle$ and $|\chi_k\rangle$. We can fix these by requiring that four of the c^{ijk} should be real: for example, we can change the phases of $|\phi_0\rangle$ and $|\phi_1\rangle$ to make c^{000} and c^{100} real, then change the phases of $|\theta_0\rangle$ and $|\theta_1\rangle$ to make c^{001} and c^{011} real, simultaneously changing the phase of $|\chi_0\rangle$ to keep c^{000} and c^{100} real. (It is easy to show that under the six-dimensional group of phase changes of the basis vectors, the generic set of coordinates has two-dimensional stabiliser, so that the orbits are four-dimensional and therefore four phases can be removed.)

From the Schmidt decompositions we obtain the one-particle density matrices

$$\begin{aligned} \rho_A &= \sum_i \alpha_i^2 |\phi_i\rangle\langle\phi_i|, \\ \rho_B &= \sum_i \beta_i^2 |\theta_i\rangle\langle\theta_i|, \\ \rho_C &= \sum_i \gamma_i^2 |\chi_i\rangle\langle\chi_i|. \end{aligned} \tag{4.5}$$

Hence the coordinates c^{ijk} satisfy

$$\begin{aligned}\sum_{jk} c^{ijk}\overline{c}_{ljk} &= \alpha_i^2\delta_l^i,\\ \sum_{ik} c^{ijk}\overline{c}_{imk} &= \beta_i^2\delta_m^j,\\ \sum_{ij} c^{ijk}\overline{c}_{ijn} &= \gamma_i^2\delta_n^k.\end{aligned} \tag{4.6}$$

To obtain a relation between the c^{ijk} and Kempe's invariant I_5, we calculate

$$\begin{aligned}&\mathrm{tr}(\rho_A\rho_B\rho_{AB})\\ &= \mathrm{tr}\left[\left(\sum_i \alpha_i^2|\phi_i\rangle_A\langle\phi_i|_A\right)\left(\sum_j \beta_j^2|\theta_j\rangle_B\langle\theta_j|_B\right)\left(\sum_k \gamma_k^2|X_k\rangle_{AB}\langle X_k|_{AB}\right)\right]\\ &= \sum_{ijk}\alpha_i^2\beta_j^2\gamma_k^2|\langle\phi_i|\theta_j|X_k\rangle|^2.\end{aligned}$$

But

$$c^{ijk} = \langle\phi_i|_A\langle\theta_j|_B\langle\chi_k|_C|\Psi\rangle = \gamma_k\langle\phi_i|_A\langle\theta_j|_B|X_k\rangle_{AB}.$$

Hence

$$\mathrm{tr}(\rho_A\rho_B\rho_{AB}) = \sum_{ijk}\alpha_i^2\beta_j^2|c^{ijk}|^2$$

and so, using (3.6),

$$I_5 = 3\sum_{ijk}\alpha_i^2\beta_j^2|c^{ijk}|^2 - \sum_i \alpha_i^6 - \sum_j \beta_j^6. \tag{4.7}$$

Finally, the relation between the c^{ijk} and the 3-tangle I_6 needs a longer argument which we will not give here. The result is

$$I_6 = \det R \tag{4.8}$$

where

$$R_j^i = (\alpha_i^4 + \alpha_i^2)\delta_j^i - \sum_{kl}(\beta_k^2 + \gamma_l^2)c^{ikl}\overline{c}_{jkl}$$

In order to determine how many states have the same values of the invariants $I_1, \ldots, I_6$, and therefore how many further discrete-valued invariants are needed to specify uniquely a pure state of three qubits up to local transformations, one would need to find the number of different sets of coordinates c^{ijk} satisfying the reality conditions given above and the equations (4.6), (4.7) and (4.8), where α_i, β_i and γ_i are determined by (4.3) and (4.4).

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